

GetBonNie for Building, Analyzing and Sharing Rule-based Models

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Short Abstract — GetBonNie is a web-based application for building, analyzing, and sharing rule-based models encoded in the BioNetGen language (BNGL). Tools accessible within the GetBonNie environment include 1) an applet for drawing graphs that correspond to BNGL code; 2) a network-generation engine for translating a set of rules into a chemical reaction network; 3) simulation engines that implement generate-first, on-the-fly, and network-free methods for simulating rule-based models; and 4) a database for sharing models, parameter values, annotations, simulation tasks and results.

Keywords — rule-based modeling, graph theory, formal language, web-based application

I. PURPOSE

THE systems-level dynamics of molecular interactions in cellular regulatory systems are difficult to model using approaches that rely on explicit specification of a chemical reaction network. The reason is combinatorial complexity [1], the potential of molecular interactions to generate large numbers of chemical species and reactions. Rule-based modeling approaches have been developed to address this problem [1]. In these approaches, molecules and molecular complexes are typically represented using graphs, or the equivalent, and molecular interactions are represented using (graph-rewriting) rules. A rule implicitly defines the reactions that can be generated by the molecular interaction that it represents.

To provide a web-based interface for various rule-based modeling software and to prompt sharing of rule-based models, we have developed GetBonNie [2].

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II. FEATURES

GetBonNie combines the capabilities of several stand-alone programs in one freely accessible web-based application. GetBonNie allows users to create rule-based models and share them within a private group or with the public. Model specifications can be either uploaded to or built *de novo* within the GetBonNie environment, which provides interactive forms to guide model building and simulations. Model specifications are automatically checked to ensure that they are well formed. GetBonNie can export models in SBML [3] format. It also includes a forum for discussing rule-based modeling.

GetBonNie provides access to simulation engines that implement stochastic and deterministic generate-first methods [4], stochastic on-the-fly methods [5], and stochastic network-free methods [6,7] for well-mixed reaction systems. When a simulation is finished, a user can plot the results online and/or download the raw simulation data.

III. CONCLUSION

GetBonNie provides a convenient web interface for rule-based modeling. In the future, we plan to extend GetBonNie to allow biological knowledge, such as protein sequences, to be linked to formal elements of models.

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